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Ab initio calculation of the NMR spin-lattice relaxation time and the diffusion coefficient of 21Ne in liquid and supercritical states

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Abstract

Molecular dynamics simulations are performed with ab initio calculated potentials and electric field gradient curves on different levels of approximation, to study their influence on the relaxation time and diffusion coefficient of fluid 21Ne. Additional properties, such as quadrupole couplings, effective electric field gradient correlation times, and diffusion correlation times, are studied to get a better understanding of the underlying mechanisms. Semi-quantitative models for the total, self and cross correlation functions of the electric field gradient are developed.